

2,2-Bis(bromomethyl)-1,3-propanediol
3296-90-0 | DTXSID9020164

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 2.34e-01 mol/L

Global applicability domain: Inside

Local applicability domain index: 5.40e-01

Confidence level: 6.17e-01

Nearest Neighbors from the Training Set

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2,2-Bis(bromomethyl)-1,3-propanediol

Measured: 1.45e-01

Predicted: 2.34e-01

Image not found

Prenderol

Measured: 1.51

Predicted: 1.04

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2-Methyl-2,4-pentanediol

Measured: 8.46

Predicted: 3.58